

USING CONCENTRATION DEPENDENCE OF MICROWAVE SPECTRA OF 2-COMPONENT MIXTURES TO IDENTIFY SINGLE COMPONENT CLUSTERS - APPLICATION TO (FLUOROETHYLENE)_n AND (1,1-DIFLUOROETHYLENE)_n

REBECCA A. PEEBLES, SEAN A. PEEBLES, PRASHANSA KANNANGARA, TULANA ARIYARATNE, *Department of Chemistry, Eastern Illinois University, Charleston, IL, USA*; BROOKS PATE, CHANNING WEST, *Department of Chemistry, The University of Virginia, Charlottesville, VA, USA*.

Over the past two years, we have implemented automated analysis of chirped-pulse microwave spectra of two-component mixtures of fluoroethylene (FE) or 1,1-difluoroethylene (DFE) and CO₂ to facilitate identification of the numerous cluster spectra present in a single scan.^a This approach has led to assignment of ten (FE)_n(CO₂)_m clusters and one (DFE)_n(CO₂)_m cluster, so far. These scans also include spectra of multiple single-component clusters (for instance, (FE)_n), which were not apparent in earlier analyses, since “monomer only” peaks were filtered from data sets during analysis. Present efforts utilize intensity variation amongst two-component scans as a way to identify these single-component clusters. Previously unobserved spectra for five clusters involving only FE or only DFE (and in some cases including neon) have now been assigned.

Identifying groups of related transitions and assigning their spectra has proven relatively straightforward, but determining compositions and structures of the carriers of these spectra is challenging. Several approaches, including analysis of the concentration dependence of transition intensity and implementation of rapid force-field based structure optimizations, have allowed some progress on determining details of the observed species.

^aRebecca A. Peebles, Prashansa B. Kannangara, Sean A. Peebles, Brooks H. Pate, 73rd International Symposium on Molecular Spectroscopy, Talk TH02, June 19, 2018.